

## Siesta 5.0.0 MPI (Open MPI)

### Webpage

<https://gitlab.com/siesta-project/siesta>

### Version

5.0.0 (+ELPA 2024.03.001, ELSI 2.9.1, NetCDF 4.9.2, NetCDF Fortran 4.6.1, libxc 6.2.2)

### Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- Intel MKL 2024.1
- Open MPI 4.1.6
- autoconf 2.72 (for ELPA)
- Python 3.9
  - ruamel.yaml (pip3.9 install ruamel.yaml --user)

### Files Required

- siesta-5.0.0.tar.gz
- netcdf-c-4.9.2.tar.gz
- netcdf-fortran-4.6.1.tar.gz
- libxc-6.2.2.tar.bz2
- elsi\_interface-v2.9.1.tar.gz
- elpa-2024.03.001.tar.gz
- wannier90-3.1.0.tar.gz
- gnu\_rccs\_ompi.cmake (for ELSI 2.9.1)

```
### GCC ###
```

```
SET(CMAKE_Fortran_COMPILER "mpif90" CACHE STRING "MPI Fortran compiler")
```

```
SET(CMAKE_C_COMPILER "mpicc" CACHE STRING "MPI C compiler")
```

```
SET(CMAKE_CXX_COMPILER "mpicxx" CACHE STRING "MPI C++ compiler")
```

```
SET(CMAKE_Fortran_FLAGS "-O3 -fallow-argument-mismatch" CACHE STRING "Fortran flags")
```

```
SET(CMAKE_C_FLAGS "-O3 -std=c99" CACHE STRING "C flags")
```

```
SET(CMAKE_CXX_FLAGS "-O3 -std=c++11" CACHE STRING "C++ flags")
```

```
SET(ENABLE_PEXSI ON CACHE BOOL "Enable PEXSI")
```

```
SET(ENABLE_TESTS ON CACHE BOOL "Enable Fortran tests")
```

```
SET(ENABLE_C_TESTS ON CACHE BOOL "Enable C tests")
```

```
SET(LIB_PATHS "$ENV{MKLRROOT}/lib/intel64" CACHE STRING "External library paths")
```

```
SET(LIBS "mkl_scalapack_lp64 mkl_gf_lp64 mkl_sequential mkl_core mkl_blacs_openmpi_lp64 m dl" CACHE STRING "External libraries")
```

### Build Procedure

#### ELSI (for PEXSI, not for ELPA)

```
#!/bin/sh
```

```
VERSION=2.9.1
```

```
INSTDIR=/apl/siesta/5.0.0/exts
```

```
BASEDIR=/home/users/${USER}/Software/ELSI/${VERSION}
```

```
TARBALL=${BASEDIR}/elsi_interface-v${VERSION}.tar.gz
```

```
WORKDIR=/gwork/users/${USER}
```

```
MYTC_NAME=gnu_rccs_ompi.cmake
```

```
MYTC=${BASEDIR}/${MYTC_NAME}
```

```
PARALLEL=24
```

```

export LANG=C
export LC_ALL=C

# -----
umask 0022
ulimit -s unlimited

cd ${WORKDIR}
if [ -d elsi_interface-v${VERSION} ]; then
  mv elsi_interface-v${VERSION} elsi-erase
  rm -rf elsi-erase &
fi

module -s purge
module -s load gcc-toolset/13
module -s load mkl/2024.1
module -s load openmpi/4.1.6/gcc13

tar xf ${TARBALL}
cd elsi_interface-v${VERSION}
cp ${MYTC} toolchains

mkdir build && cd build
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTDIR} \
  -DCMAKE_TOOLCHAIN_FILE=../toolchains/${MYTC_NAME} \
  -DBUILD_SHARED_LIBS=ON

make -j ${PARALLEL}
make test
make install

```

## ELPA

```

#!/bin/sh

ELPA_VERSION=2024.03.001
INSTDIR=/apl/siesta/5.0.0/elpa
WORKDIR=/gwork/users/${USER}

BASEDIR=/home/users/${USER}/Software/ELPA/${ELPA_VERSION}
TARBALL=${BASEDIR}/elpa-${ELPA_VERSION}.tar.gz

PARALLEL=12

# -----
umask 0022
ulimit -s unlimited

module -s purge
module -s load gcc-toolset/13
module -s load mkl/2024.1
module -s load openmpi/4.1.6/gcc13
module -s load autoconf/2.72

export LANG=C
export LC_ALL=C

export FC=mpif90
export CC=mpicc
export CXX=mpicxx
export CFLAGS="-march=znver3"
# mkl_link_tool -opts -c gnu_f -p no --cluster_library=scalapack -m openmpi
export FCFLAGS="-m64 -I${MKLRROOT}/include"
# mkl_link_tool -libs -c gnu_f -p no --cluster_library=scalapack -m openmpi
export LDFLAGS="-L${MKLRROOT}/lib -lmkl_scalapack_lp64 -Wl,--no-as-needed -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lmkl_blacs_openmpi_lp64 -lpthread -lm -ldl"

```

```

cd ${WORKDIR}
if [ -d elpa-${ELPA_VERSION} ]; then
  mv elpa-${ELPA_VERSION} elpa-erase
  rm -rf elpa-erase &
fi
tar zxf ${TARBALL}
cd elpa-${ELPA_VERSION}

./configure --prefix=${INSTDIR} \
  --disable-avx512-kernels
make -j ${PARALLEL}
make check
make install

```

## Siesta

```

#!/bin/sh

SIESTA_VERSION=5.0.0
INSTDIR=/apl/siesta/5.0.0

WORKDIR=/gwork/users/${USER}
BASEDIR=/home/users/${USER}/Software/Siesta/${SIESTA_VERSION}
TARBALL=${BASEDIR}/siesta-${SIESTA_VERSION}.tar.gz

NETCDF_C_VERSION=4.9.2
NETCDF_F_VERSION=4.6.1
BASEDIR_NETCDF=/home/users/${USER}/Software/NETCDF
TARBALL_NETCDF_C=${BASEDIR_NETCDF}/c${NETCDF_C_VERSION}/netcdf-c-${NETCDF_C_VERSION}.tar.gz
TARBALL_NETCDF_F=${BASEDIR_NETCDF}/f${NETCDF_F_VERSION}/netcdf-fortran-${NETCDF_F_VERSION}.tar.gz
WANNIER90_VERSION=3.1.0
BASEDIR_WANNIER90=/home/users/${USER}/Software/wannier90/${WANNIER90_VERSION}
TARBALL_WANNIER90=${BASEDIR_WANNIER90}/wannier90-${WANNIER90_VERSION}.tar.gz

LIBXC_VERSION=6.2.2
BASEDIR_LIBXC=/home/users/${USER}/Software/libxc
TARBALL_LIBXC=${BASEDIR_LIBXC}/${LIBXC_VERSION}/libxc-${LIBXC_VERSION}.tar.bz2

PARALLEL=12

#-----
umask 0022
ulimit -s unlimited

module -s purge
module -s load gcc-toolset/13
module -s load mkl/2024.1
module -s load openmpi/4.1.6/gcc13

export LANG=C
export LC_ALL=C
export OMP_NUM_THREADS=1

# netcdf-c

cd ${WORKDIR}
if [ -d netcdf-c-${NETCDF_C_VERSION} ]; then
  mv netcdf-c-${NETCDF_C_VERSION} netcdf-c-erase
  rm -rf netcdf-c-erase &
fi
tar zxf ${TARBALL_NETCDF_C}
cd netcdf-c-${NETCDF_C_VERSION}

./configure --prefix=${INSTDIR}/exts
make -j${PARALLEL}
make -j${PARALLEL} check
make install

```

```

export PATH="${INSTDIR}/exts/bin:${PATH}"
export CPATH="${INSTDIR}/exts/include:${CPATH}"
export LD_LIBRARY_PATH="${INSTDIR}/exts/lib:${LD_LIBRARY_PATH}"
export LIBRARY_PATH="${INSTDIR}/exts/lib:${LIBRARY_PATH}"

# netcdf-f

cd ${WORKDIR}
if [ -d netcdf-fortran-${NETCDF_F_VERSION} ]; then
  mv netcdf-fortran-${NETCDF_F_VERSION} netcdf-fortran-erase
  rm -rf netcdf-fortran-erase &
fi
tar xzf ${TARBALL_NETCDF_F}
cd netcdf-fortran-${NETCDF_F_VERSION}

LDFLAGS="-L${INSTDIR}/exts/lib" \
  ./configure --prefix=${INSTDIR}/exts
make -j${PARALLEL}
make -j${PARALLEL} check
make install

# libxc

cd ${WORKDIR}
if [ -d libxc-${LIBXC_VERSION} ]; then
  mv libxc-${LIBXC_VERSION} libxc-erase
  rm -rf libxc-erase &
fi
tar xf ${TARBALL_LIBXC}
cd libxc-${LIBXC_VERSION}
autoreconf -i
./configure --prefix=${INSTDIR}/exts
make -j24
make -j24 check
make install

# siesta

cd ${WORKDIR}
rm -rf netcdf-fortran-${NETCDF_F_VERSION} \
  netcdf-c-${NETCDF_C_VERSION} \
  libxc-${LIBXC_VERSION} &

if [ -d siesta-${SIESTA_VERSION} ]; then
  mv siesta-${SIESTA_VERSION} siesta-erase
  rm -rf siesta-erase
fi

tar xzf ${TARBALL}
cd siesta-${SIESTA_VERSION}

unset CC
unset FC
export WANNIER90_PACKAGE=${TARBALL_WANNIER90}

mkdir build && cd build
cmake .. \
  -DCMAKE_INSTALL_PREFIX="${INSTDIR}" \
  -DCMAKE_PREFIX_PATH="${INSTDIR}/elpa:${INSTDIR}/exts" \
  -DCMAKE_C_COMPILER=mpicc \
  -DCMAKE_Fortran_COMPILER=mpif90 \
  -DPython3_EXECUTABLE=/usr/bin/python3.9 \
  -DSIESTA_WITH_MPI=ON \
  -DNetCDF_ROOT="${INSTDIR}/exts" \
  -DLAPACK_LIBRARY="-m64 -L${MKLRROOT}/lib -Wl,--no-as-needed -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl" \
  -DBLAS_LIBRARY="-m64 -L${MKLRROOT}/lib -Wl,--no-as-needed -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl" \
  -DSCALAPACK_LIBRARY="-lmkl_scalapack_lp64 -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lmkl_blacs_openmpi_lp64 -lpthread -lm -ldl" \

```

```
-DSIESTA_WITH_WANNIER90=ON \  
-DSIESTA_WITH_ELPA=ON \  
-DSIESTA_WITH_PEXSI=ON  
  
make -j ${PARALLEL}  
SIESTA_TESTS_VERIFY=1 ctest  
make install  
  
cd ../  
cp -r Examples ${INSTDIR}
```

## Tests

### ELSI

Passed all the tests.

### ELPA

Following tests failed.

- FAIL: validate\_c\_version\_complex\_double\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_c\_version\_real\_double\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_c\_version\_complex\_single\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_c\_version\_real\_single\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_c\_version\_complex\_double\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_c\_version\_complex\_double\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_c\_version\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_c\_version\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_c\_version\_complex\_single\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_c\_version\_complex\_single\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_c\_version\_real\_single\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_c\_version\_real\_single\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_cpp\_version\_complex\_double\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_cpp\_version\_real\_double\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_cpp\_version\_complex\_single\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_cpp\_version\_real\_single\_eigenvalues\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_cpp\_version\_complex\_double\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_cpp\_version\_complex\_double\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_cpp\_version\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_cpp\_version\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_cpp\_version\_complex\_single\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_cpp\_version\_real\_single\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_cpp\_version\_real\_single\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_real\_double\_eigenvectors\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_real\_single\_eigenvectors\_2stage\_default\_kernel\_analytic\_default.sh
- FAIL: validate\_real\_double\_eigenvectors\_2stage\_default\_kernel\_frank\_default.sh
- FAIL: validate\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_split\_comm\_myself\_explicit\_default.sh
- FAIL: validate\_real\_double\_eigenvectors\_2stage\_default\_kernel\_random\_split\_comm\_myself\_default.sh
- FAIL: validate\_real\_single\_eigenvectors\_2stage\_default\_kernel\_random\_explicit\_default.sh
- FAIL: validate\_real\_single\_eigenvectors\_2stage\_default\_kernel\_random\_default.sh
- FAIL: validate\_real\_double\_eigenvectors\_2stage\_default\_kernel\_toeplitz\_default.sh
- FAIL: validate\_real\_single\_eigenvectors\_2stage\_default\_kernel\_toeplitz\_default.sh
- FAIL: validate\_complex\_2stage\_banded\_default.sh
- FAIL: validate\_single\_complex\_2stage\_banded\_default.sh

### Siesta

(All the netcdf and libxc tests have passed.)

For Siesta, following tests failed with numerical error. Most ones are minor error. Although some of errors are bit large, changing compilers etc. could not improve the result.

- 61 - siesta-02.SpinPolarization-fe\_spin\_mpi4[verify] (Failed)
- 63 - siesta-02.SpinPolarization-fe\_spin\_directphi\_mpi4[verify] (Failed)
- 67 - siesta-02.SpinPolarization-fe\_noncol\_gga\_mpi4[verify] (Failed)

- 71 - siesta-02.SpinPolarization-fe\_noncol\_sp\_mpi4[verify] (Failed)
- 73 - siesta-03.SpinOrbit-FePt-X-X\_mpi4[verify] (Failed)
- 87 - siesta-04.SCFMixing-chargemix\_mpi4[verify] (Failed)
- 127 - siesta-08.GeometryOptimization-broyden\_vc\_mpi4[verify] (Failed)

Test logs are copied to /apl/siesta/5.0.0/test\_results.

## Notes

- We didn't try OpenMP version.
- If Intel Compiler is employed, the number of failed tests of siesta increases significantly. (Most of them are minor numerical errors, though.) Also, no significant performance improvement is observed. We thus employed gcc13.
  - In case of AMD CPU, -xHost option caused problem upon compilation. You may need to modify "-xHost" in "Config/cmake/toolchains/intel.cmake" to "-march=core-avx2" when you employ Intel Compiler.
  - icx+ifort works fine. icx+ifx couldn't complete the build.
- When large number of processes with Intel MPI, job sometimes failed with error like "Bad DM normalization: Qtot, Tr[D\*S] = 548.00000000 548.00983099". We thus employ Open MPI.
  - This error is confirmed with Examples/Carbon\_Nanoscroll input with 64 MPI processes. Open MPI version is free from this issue.
  - For small calculations (4 or 8 processes), there is no problem.
  - Intel MPI version is tentatively available. Gcc11 is used. (GCC 13 is not available.)
  - This error occurred in various versions of Intel MPI (2021.5.1 - 2021.12).
- Message like "&m -- Max memory after compute\_DM 166.26" is shown in the log file when PEXSI is enabled.
  - The memory value seems to be increasing during SCF...
- It is not easy to use ELPA in ELSI. We thus installed ELPA to the different directory.
- Python environment is necessary to do numerical verification for siesta.
  - The necessary package "ruamel.yaml" was installed with "pip3.9 install ruamel.yaml --user".
  - System python (version 3.6) can't be used for this purpose, since the test code expects Python 3.8 or later.
    - This is due to the "missing\_ok" flag for "unlink" method of Pathlib. (It might work with python 3.6 if the missing\_ok flag was removed, but we haven't tested it.)
  - CMake sometimes found out the non-default version of python3. We simply specify python 3.9 with cmake option this case.